Supporting Information

Reverse docking

The protein structure data utilized in this study were sourced from the PDBbind database, comprising a total of 17654 entries. Reverse docking was executed using Glide Dock, a specialized docking program developed by Schrödinger. The resulting analysis identified the top 50 structures, ranked based on their highest docking scores, as outlined below:

Table S1 Top 50 docking score of reverse docking.

Num.	PDB	Docking score
1	5f1j	-16.97
2	5mym	-15.97
3	5ioy	-15.82
4	4csj	-15.35
5	3hfj	-14.61
6	4hvs	-14.60
7	3mlb	-14.49
8	5ipa	-14.41
9	4m3e	-13.86
10	3n7h	-13.80
11	4ymj	-13.79
12	3k22	-13.79
13	5ezh	-13.79
14	3g08	-13.76
15	4pms	-13.71
16	6c0n	-13.71
17	3k84	-13.67
18	6fni	-13.66
19	5f0h	-13.66
20	2ofv	-13.64
21	3qri	-13.62
22	4ono	-13.59
23	4mxc	-13.57
24	5mo8	-13.56
25	4ckr	-13.54

Num.	PDB	Docking score
26	4ckr	-13.54
27	1fm9	-13.52
28	5vqx	-13.52
29	5vqt	-13.50
30	3are	-13.49
31	2hz0	-13.48
32	5m7m	-13.43
33	2og8	-13.42
34	3ctq	-13.41
35	4m3f	-13.41
36	5q15	-13.39
37	4m3d	-13.34
38	5vqq	-13.32
39	4dlj	-13.29
40	5f04	-13.27
41	4m3b	-13.24
42	3fun	-13.19
43	2vj8	-13.18
44	4at4	-13.18
45	4omk	-13.16
46	5yqo	-13.15
47	5vqr	-13.14
48	3ftz	-13.14
49	4i5h	-13.13
50	3ugc	-13.13

^{1}H, ^{13}C NMR and HRMS spectra

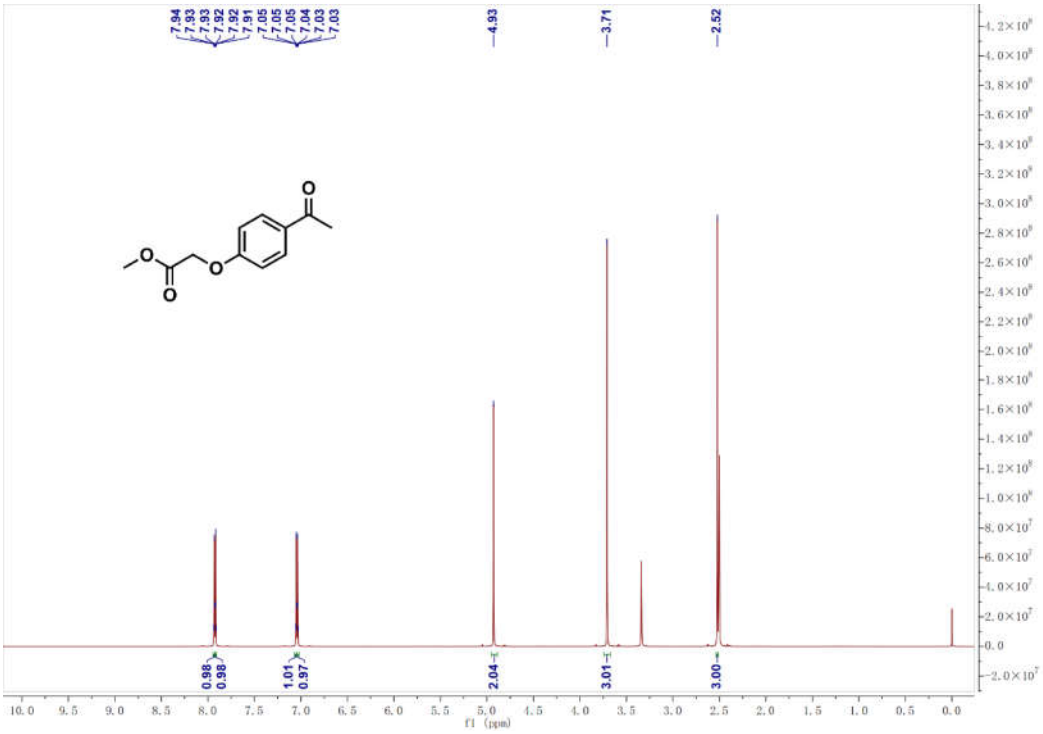

Figure S1. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound 1

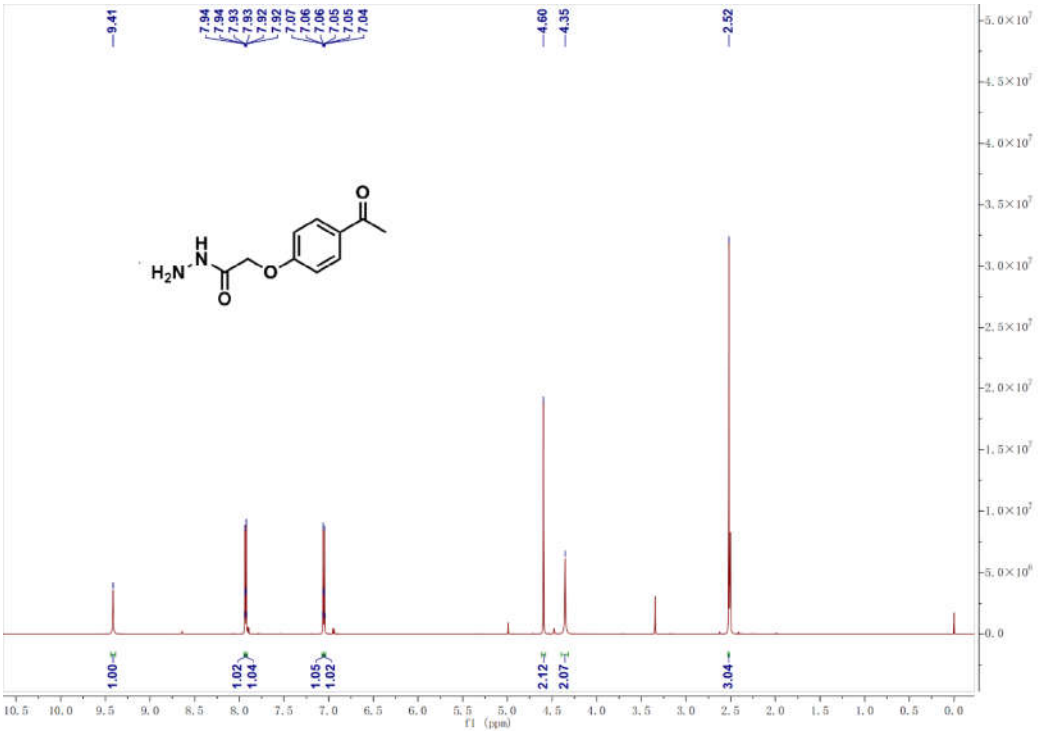

Figure S2. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound 2

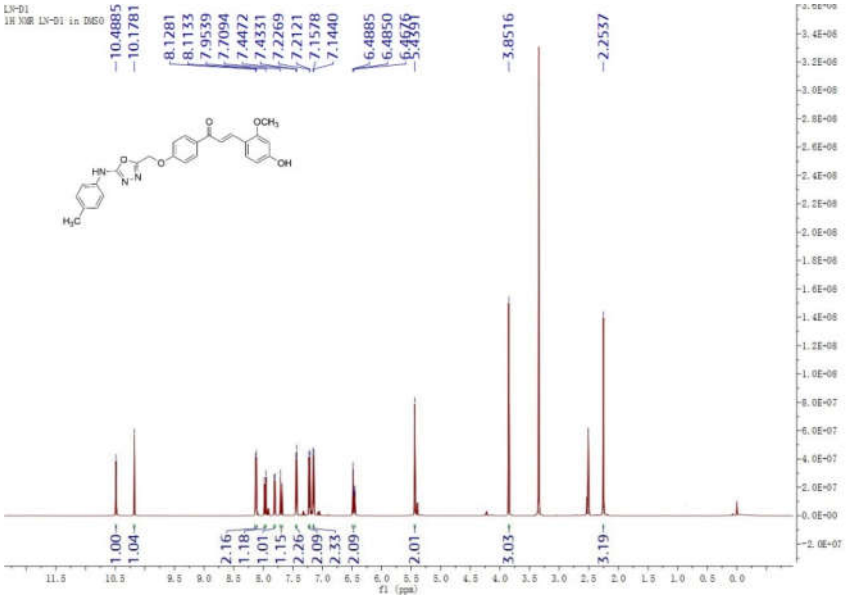

Figure S3. ^{1}H NMR (600 MHz, DMSO-*d*$_6$) spectrum of compound T1

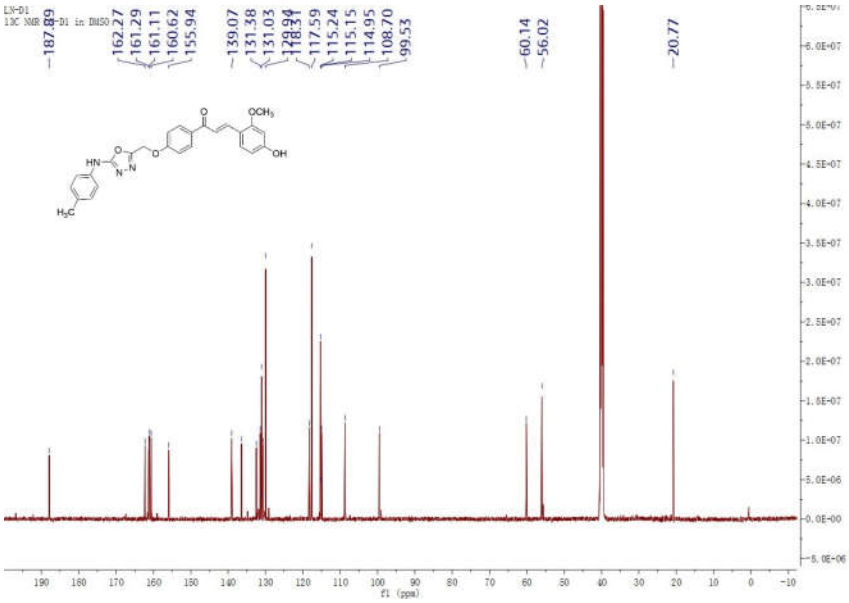

Figure S4. ^{13}C NMR (150 MHz, DMSO-*d*$_6$) spectrum of compound T1

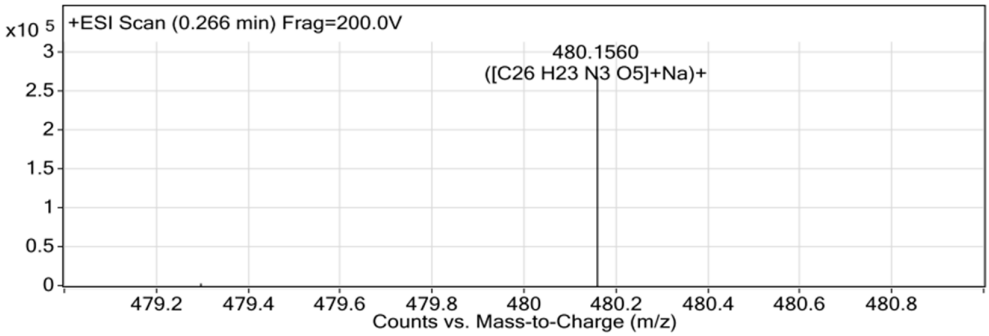

Figure S5. Mass spectrum of compound T1

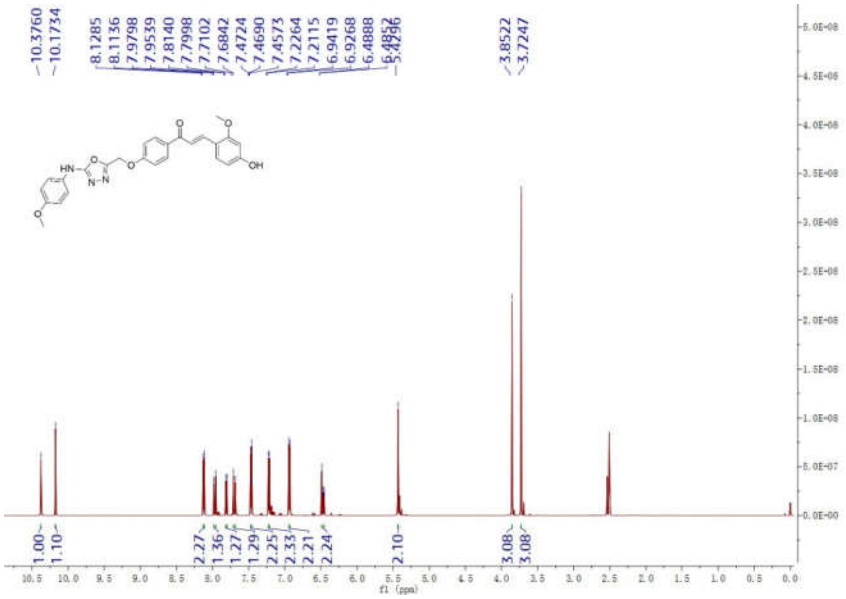

Figure S6. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T2

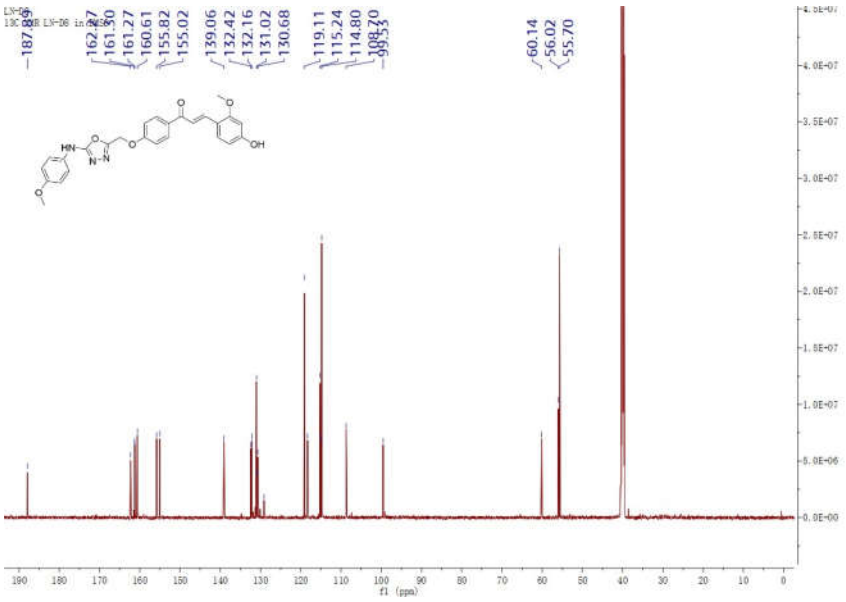

Figure S7. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T2

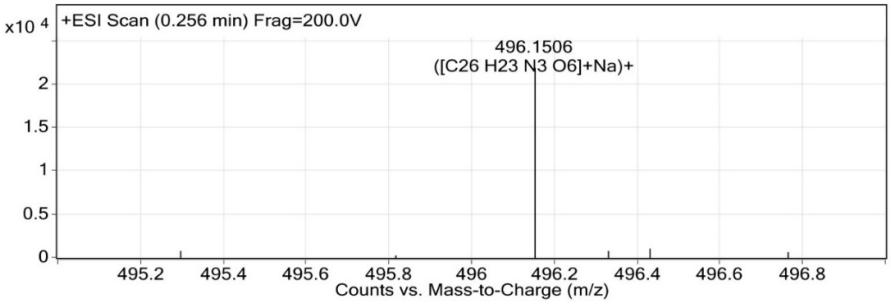

Figure S8. Mass spectrum of compound T2

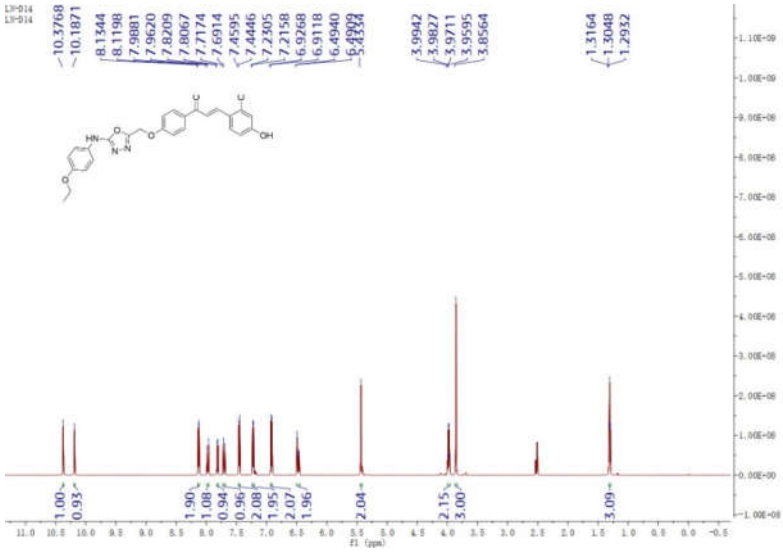

Figure S9. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T3

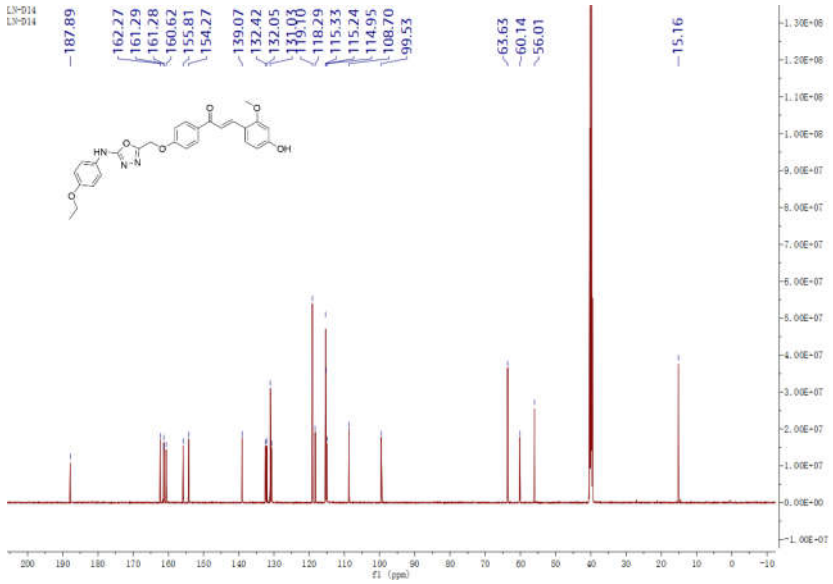

Figure S10. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T3

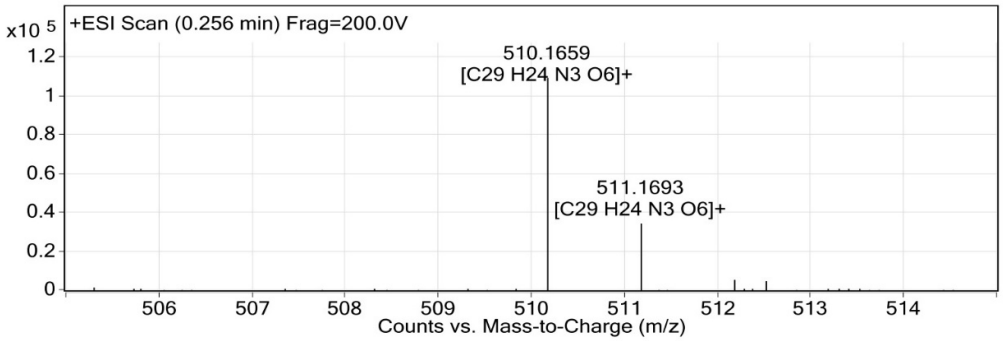

Figure S11. Mass spectrum of compound T3

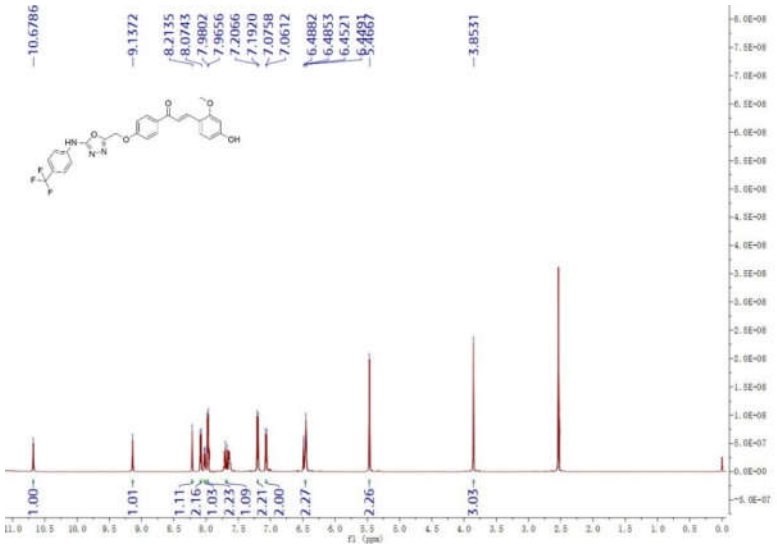

Figure S12. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T4

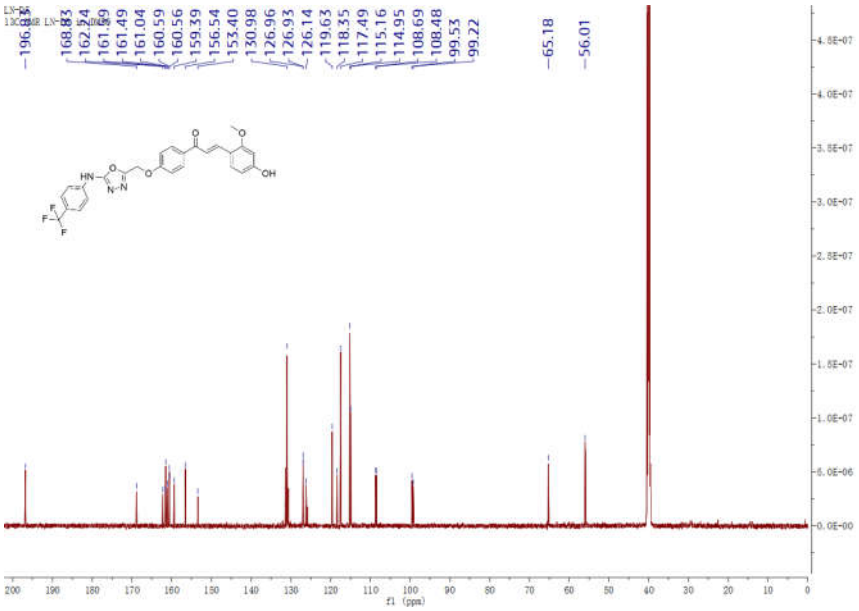

Figure S13. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T4

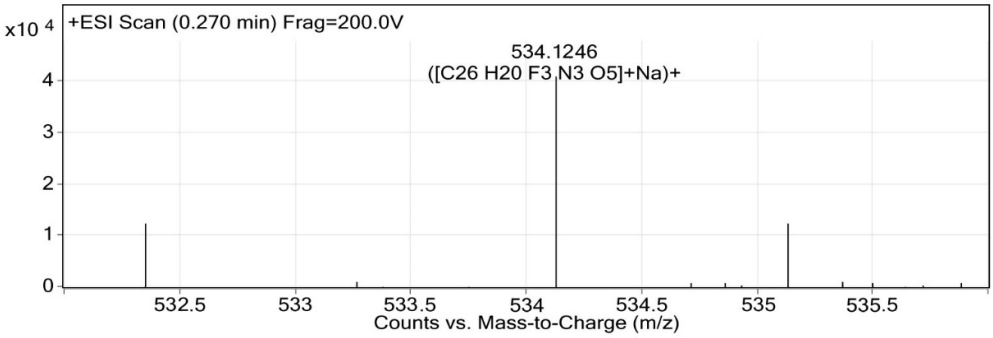

Figure S14. Mass spectrum of compound T4

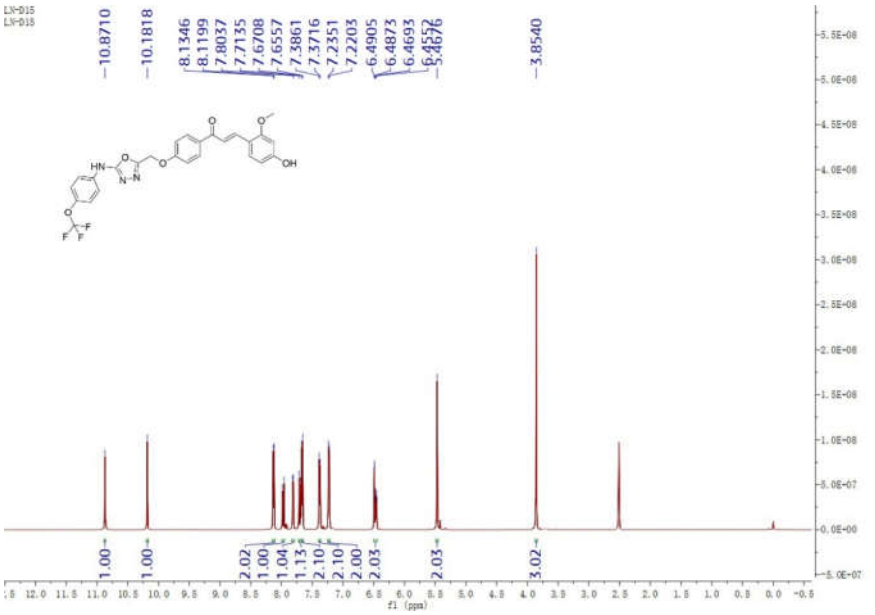

Figure S15. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T5

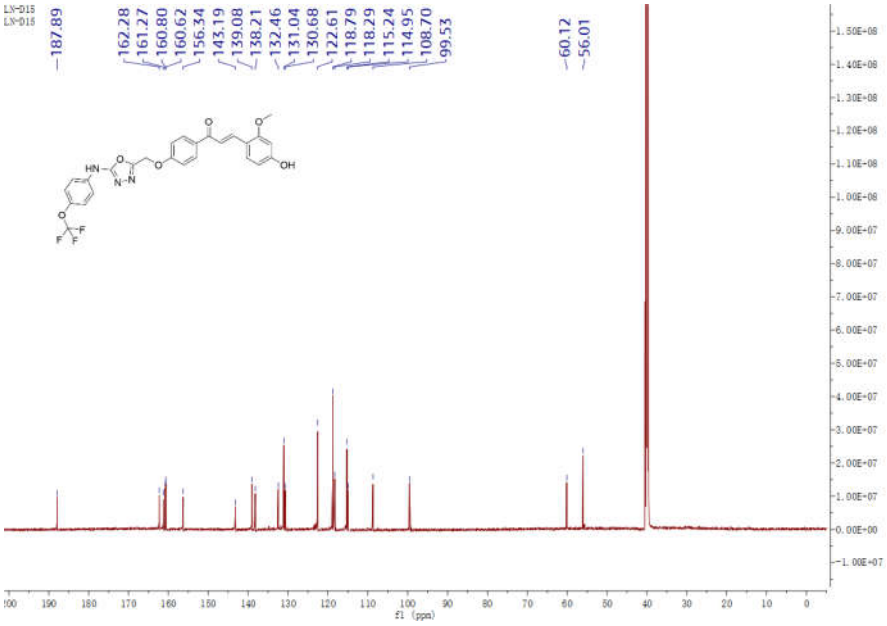

Figure S16. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T5

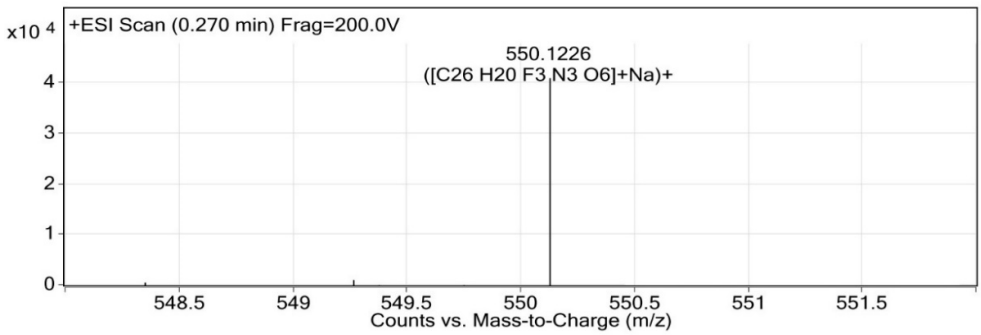

Figure S17. Mass spectrum of compound T5

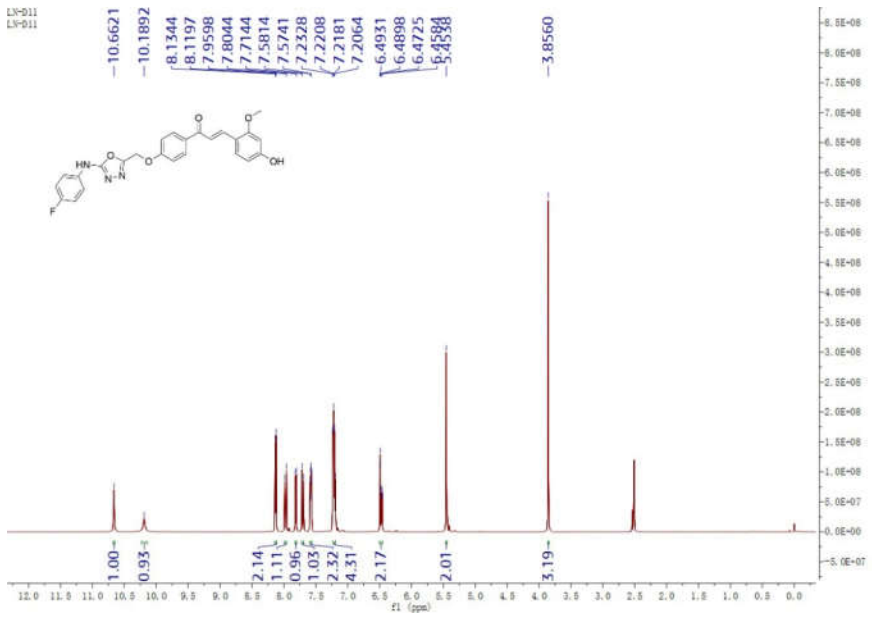

Figure S18. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T6

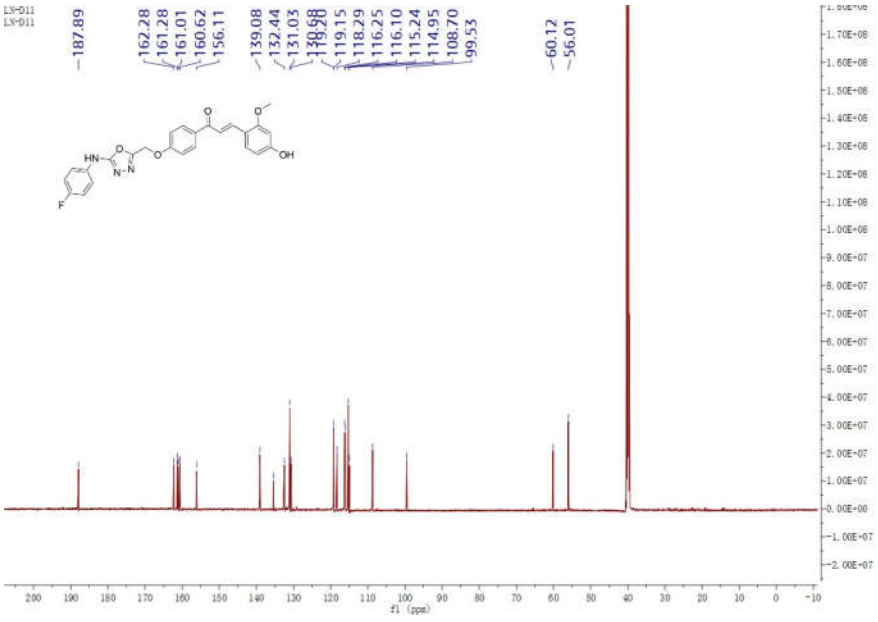

Figure S19. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T6

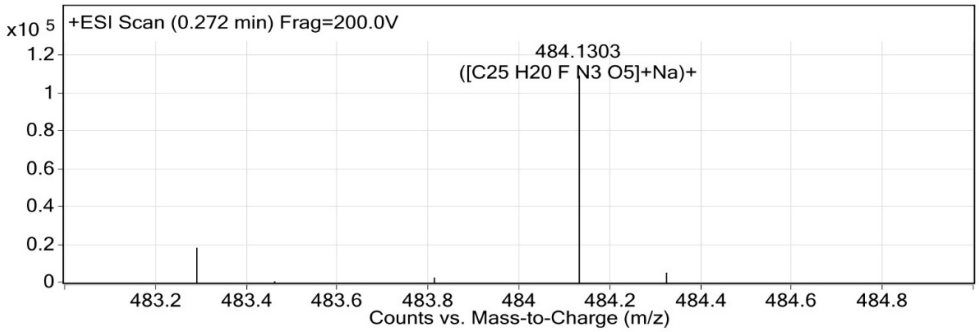

Figure S20. Mass spectrum of compound T6

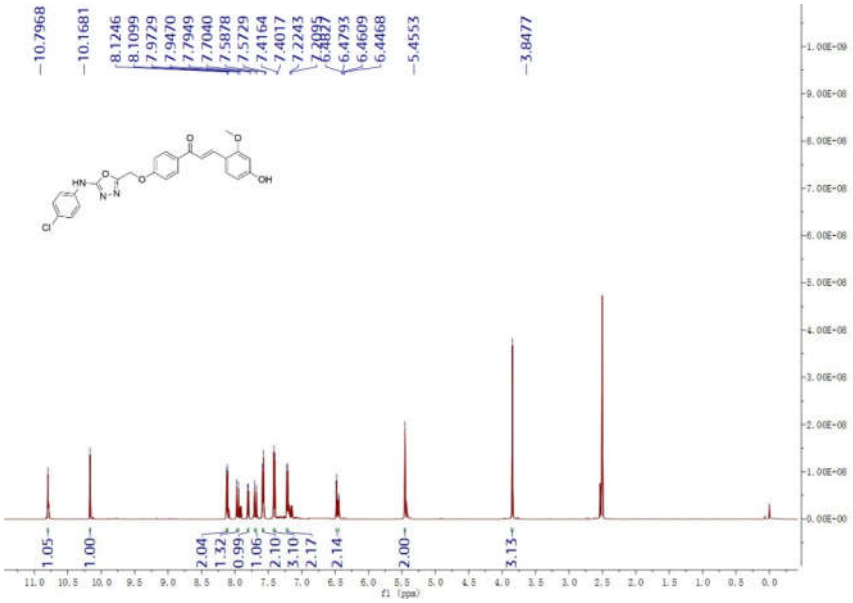

Figure S21. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T7

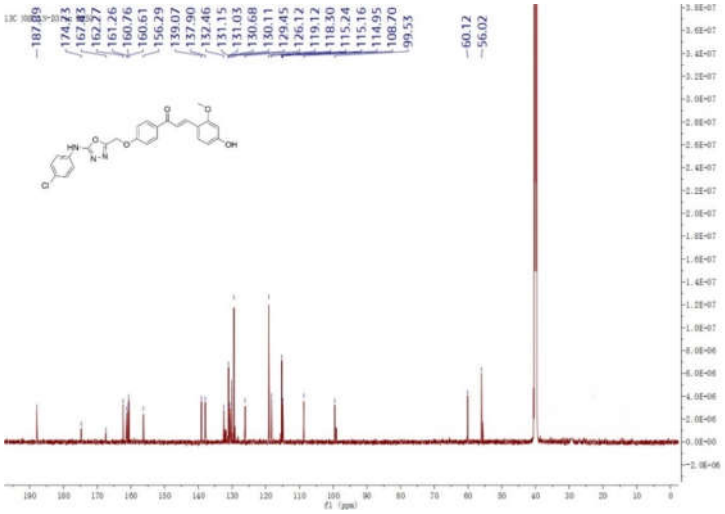

Figure S22. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T7

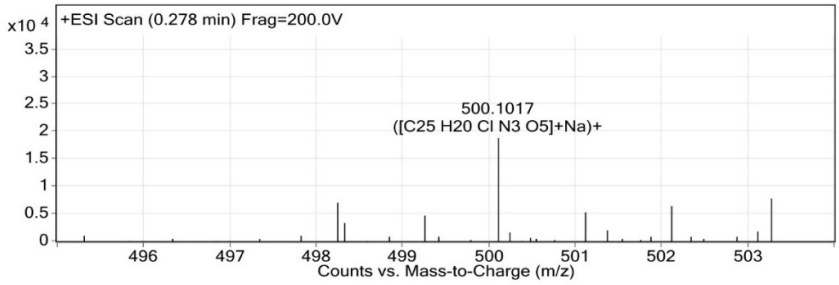

Figure S23. Mass spectrum of compound T7

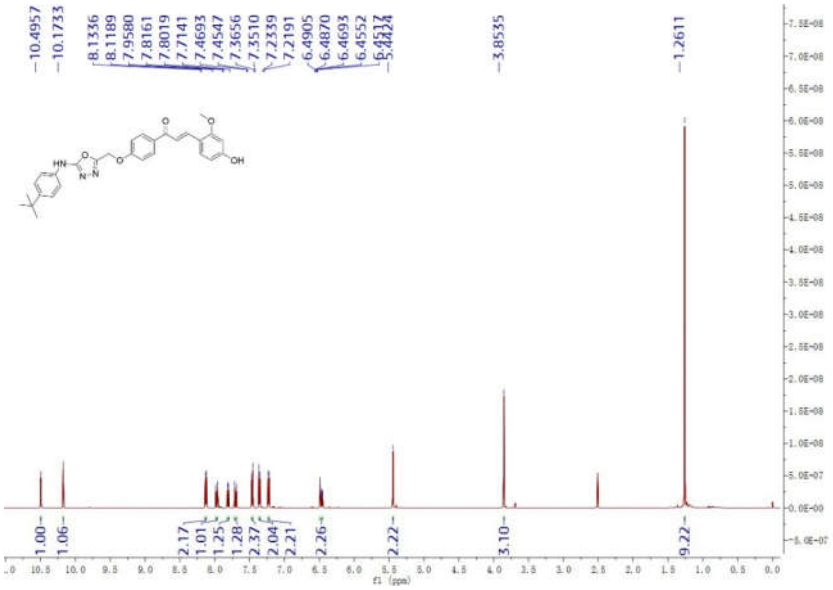

Figure S24. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T8

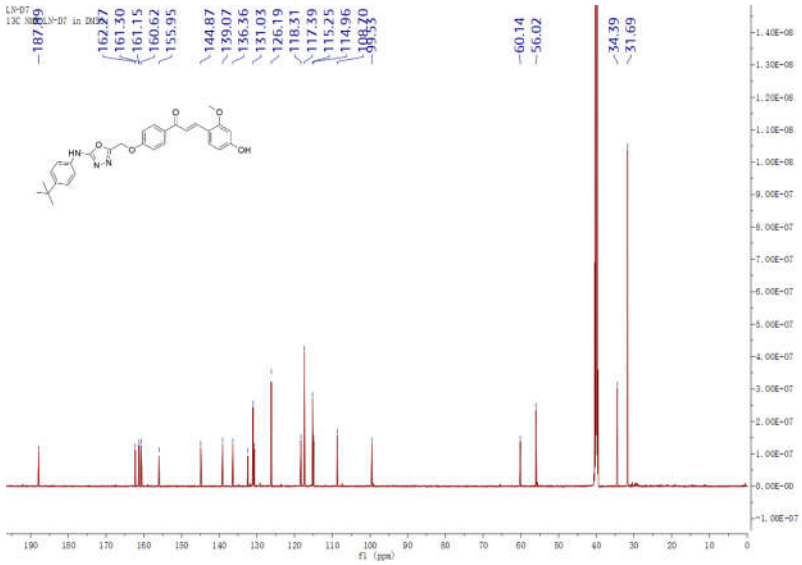

Figure S25. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T8

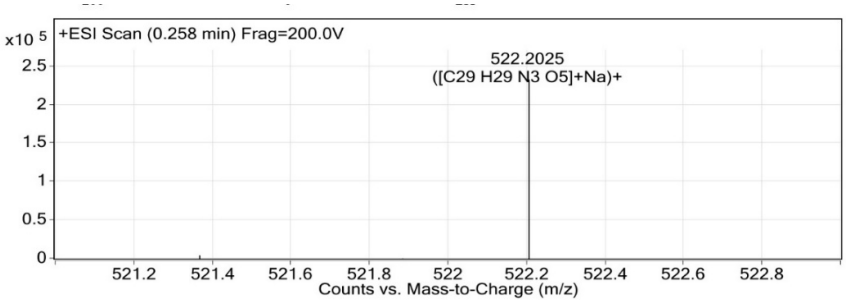

Figure S26. Mass spectrum of compound T8

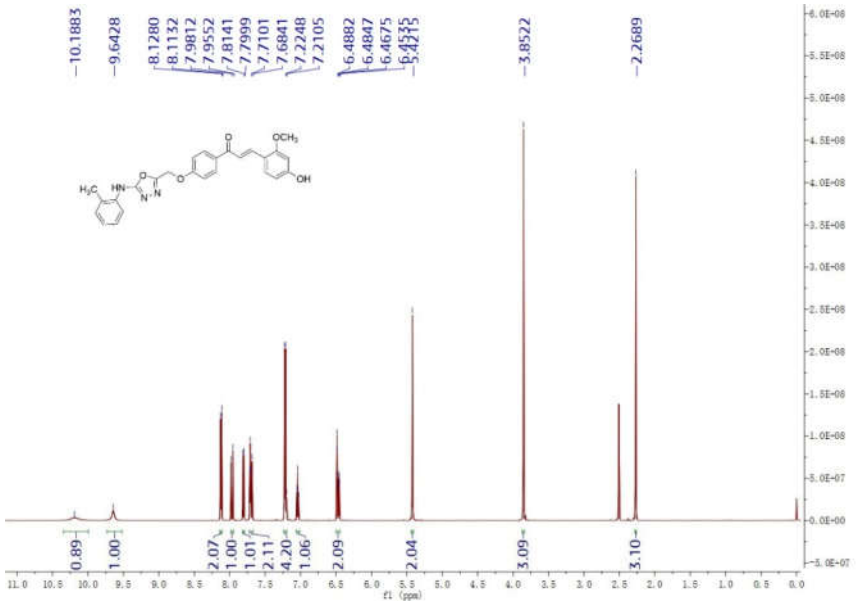

Figure S27. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T9

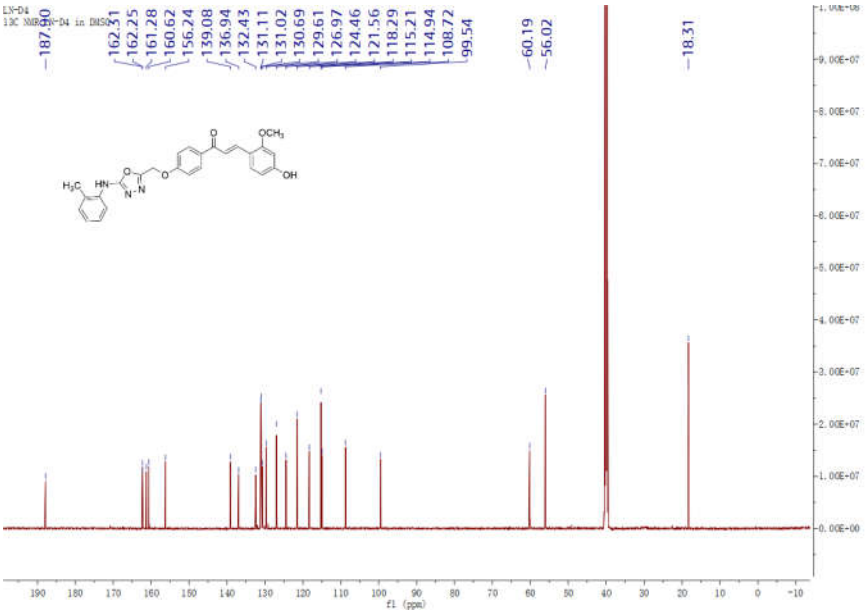

Figure S28. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T9

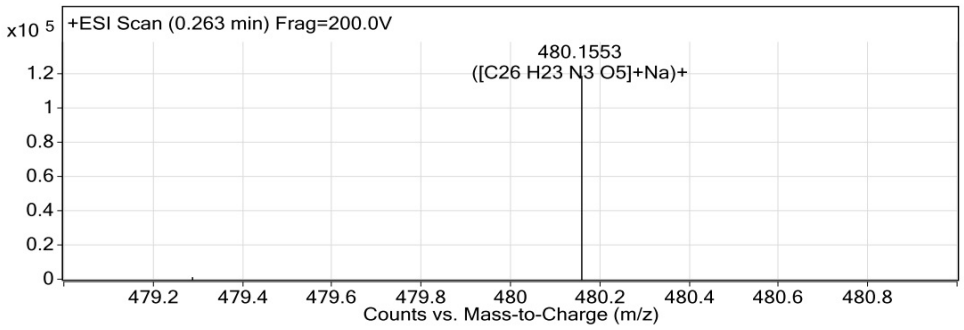

Figure S29. Mass spectrum of compound T9

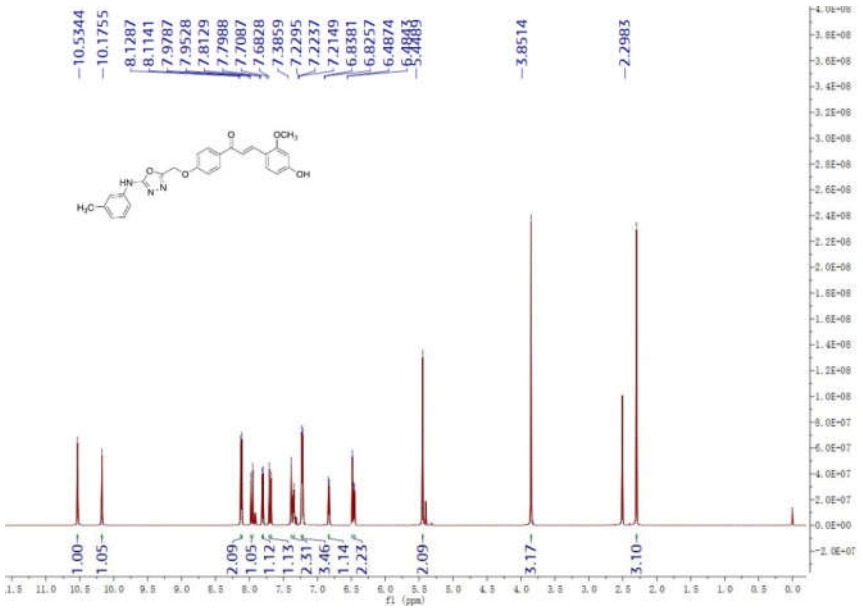

Figure S30. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T10

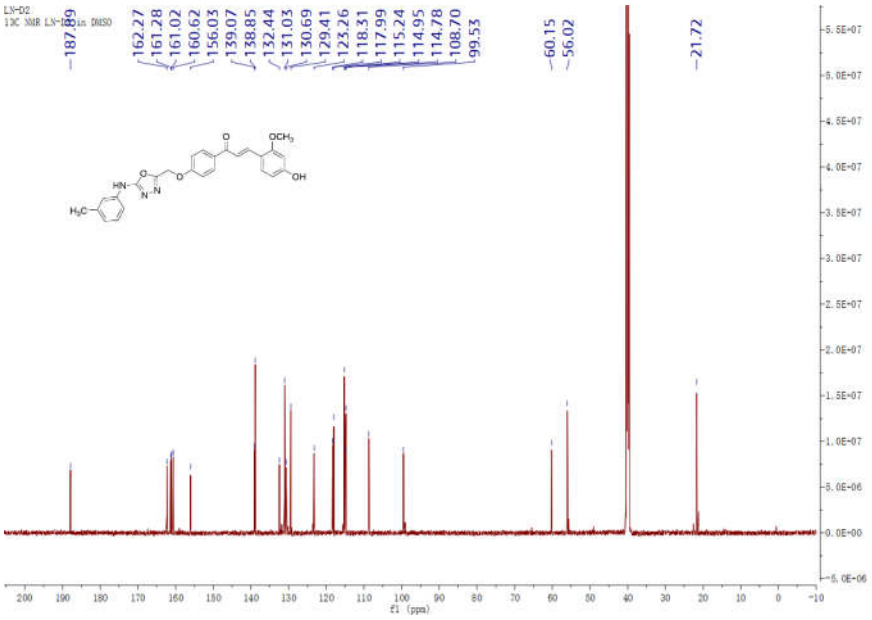

Figure S31. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T10

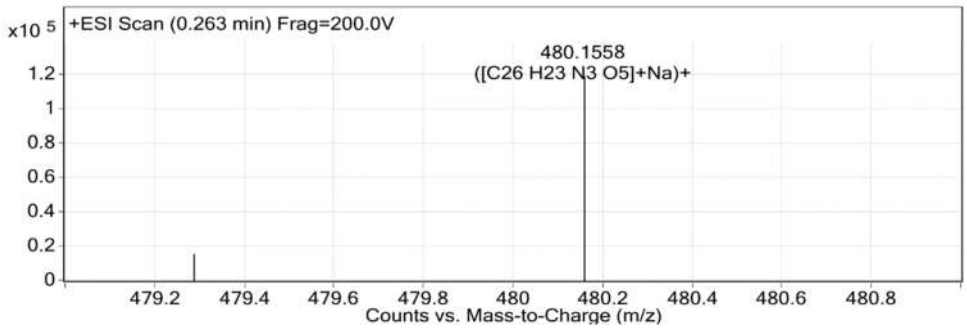

Figure S32. Mass spectrum of compound T10

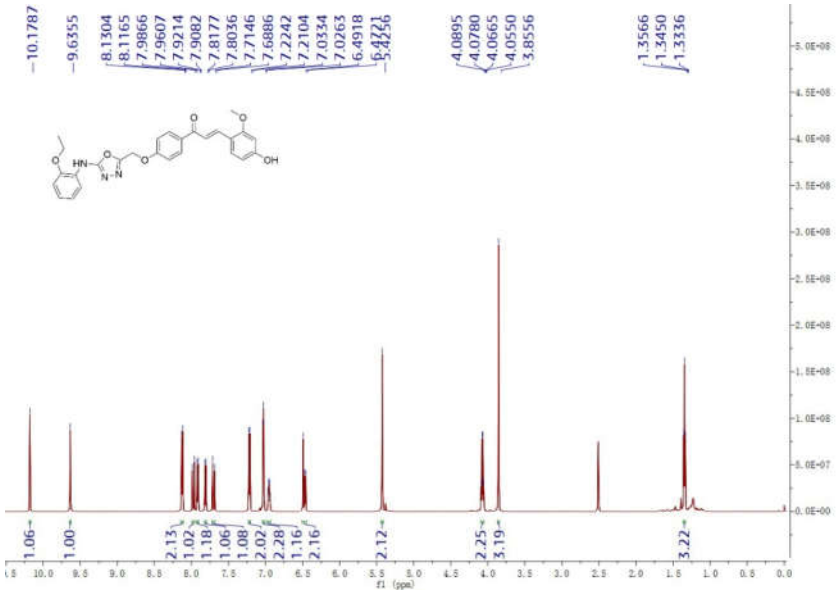

Figure S33. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T11

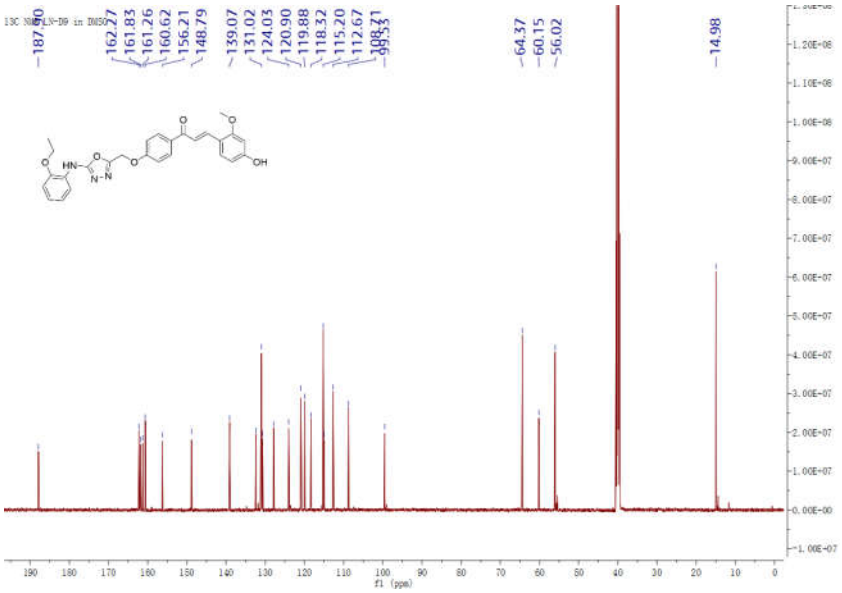

Figure S34. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T11

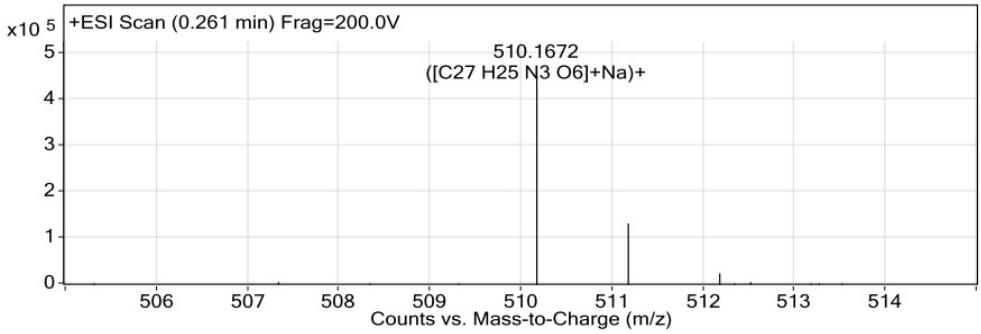

Figure S35. Mass spectrum of compound T11

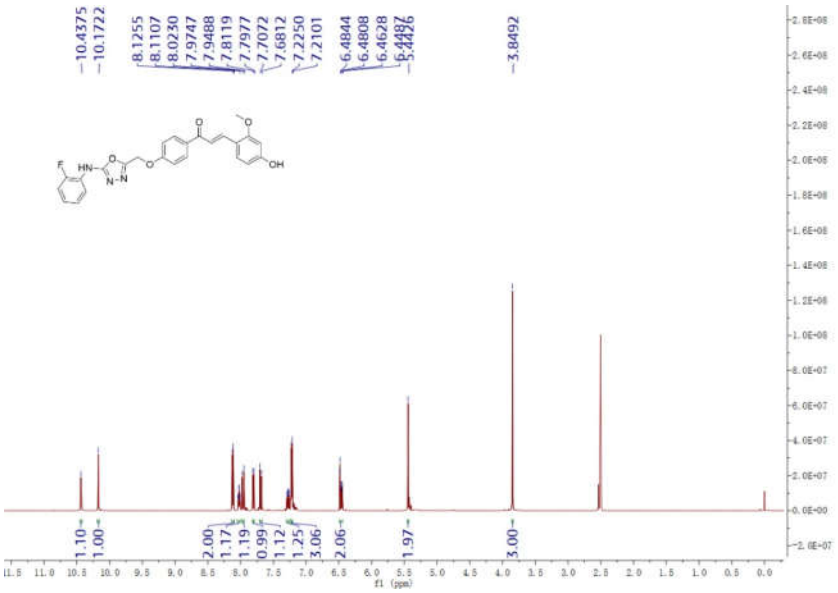

Figure S36. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T12

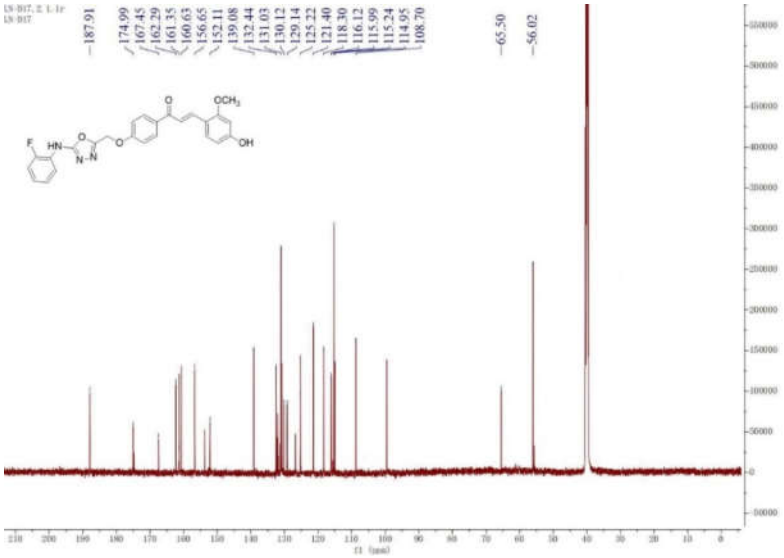

Figure S37. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T12

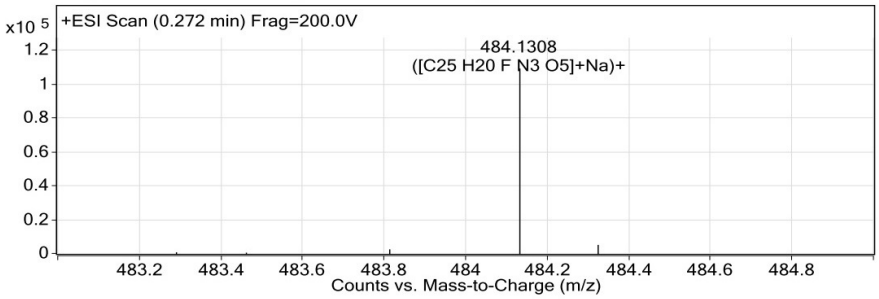

Figure S38. Mass spectrum of compound T12

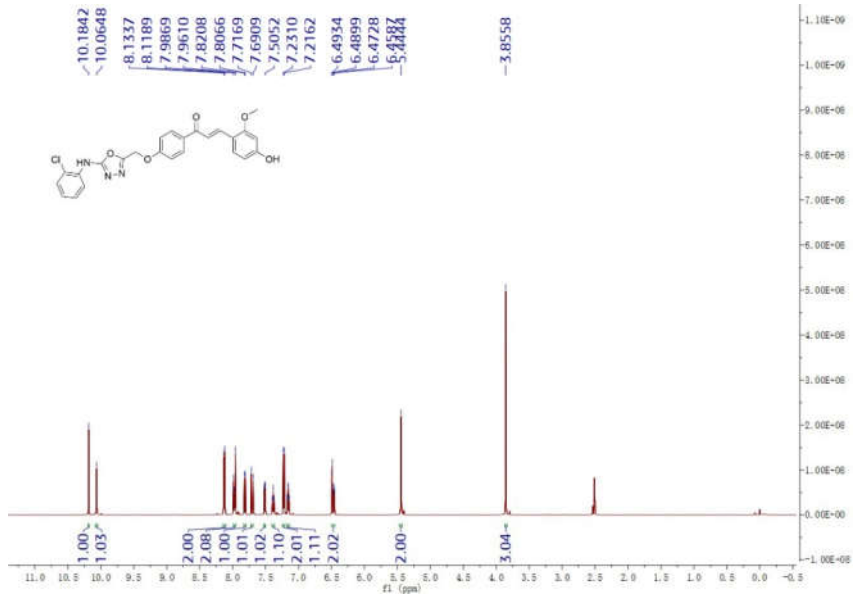

Figure S39. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T13

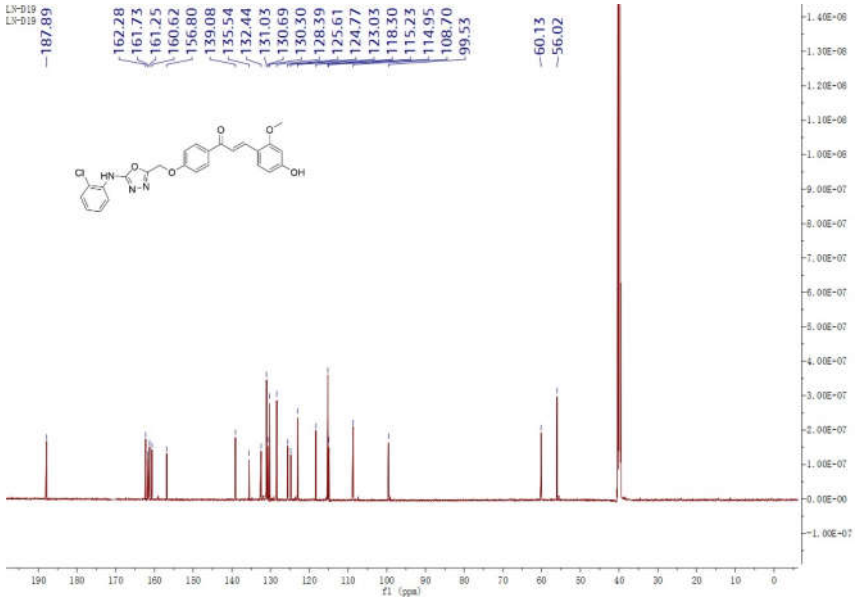

Figure S40. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T13

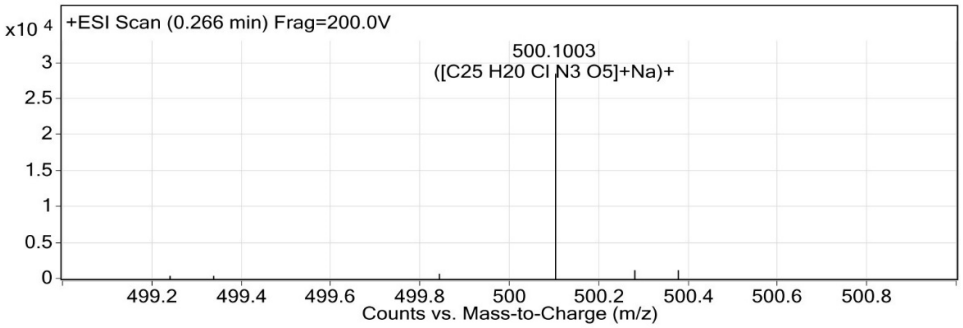

Figure S41. Mass spectrum of compound T13

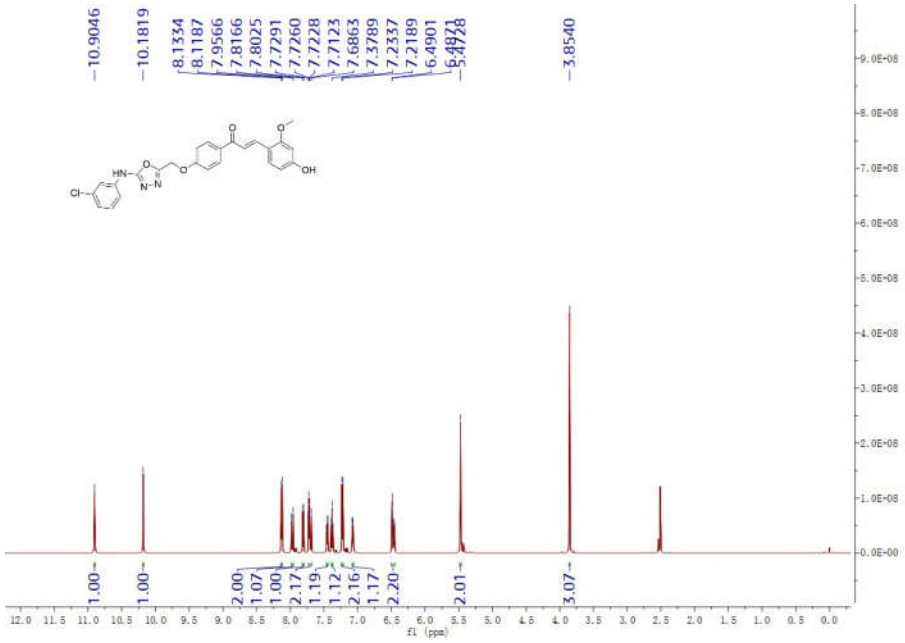

Figure S42. ^{1}H NMR (600 MHz, DMSO-*d*$_6$) spectrum of compound T14

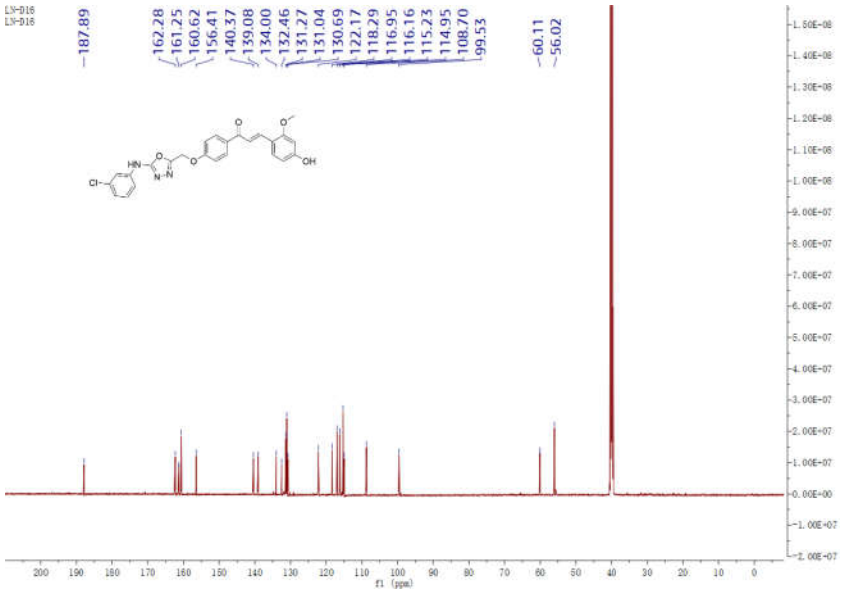

Figure S43. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T14

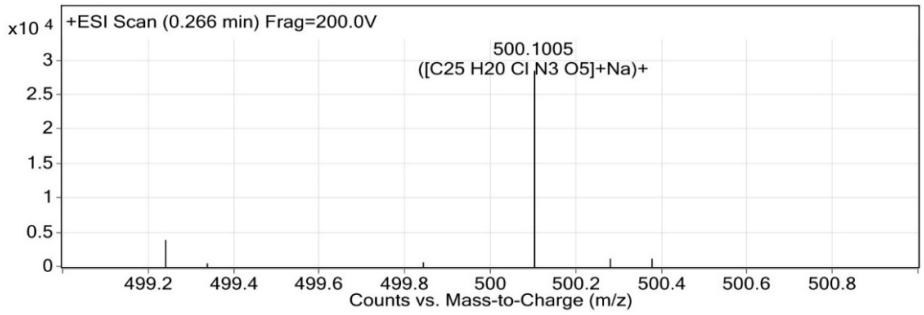

Figure S44. Mass spectrum of compound T14

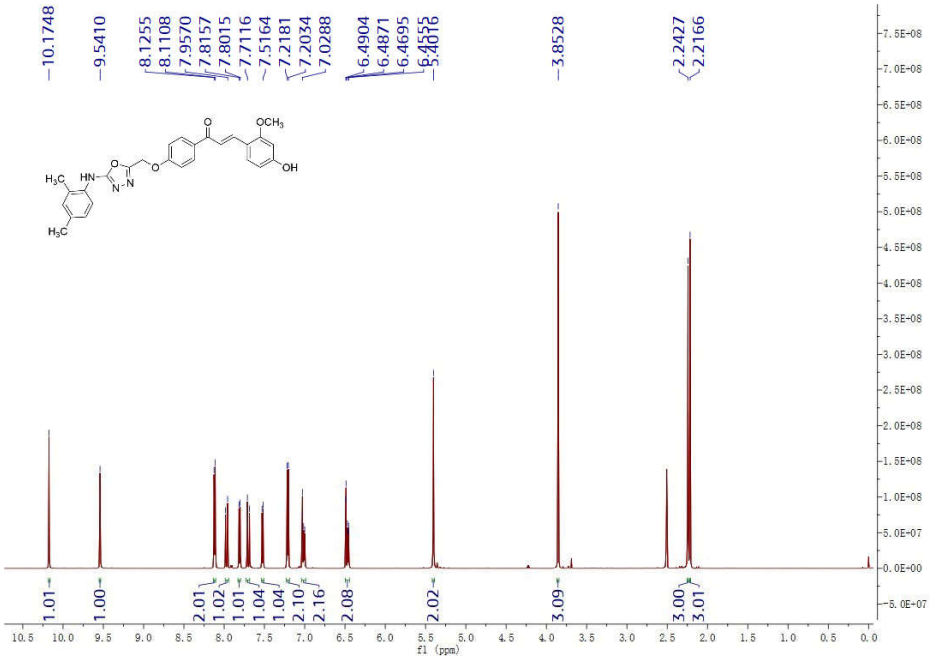

Figure S45. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T15

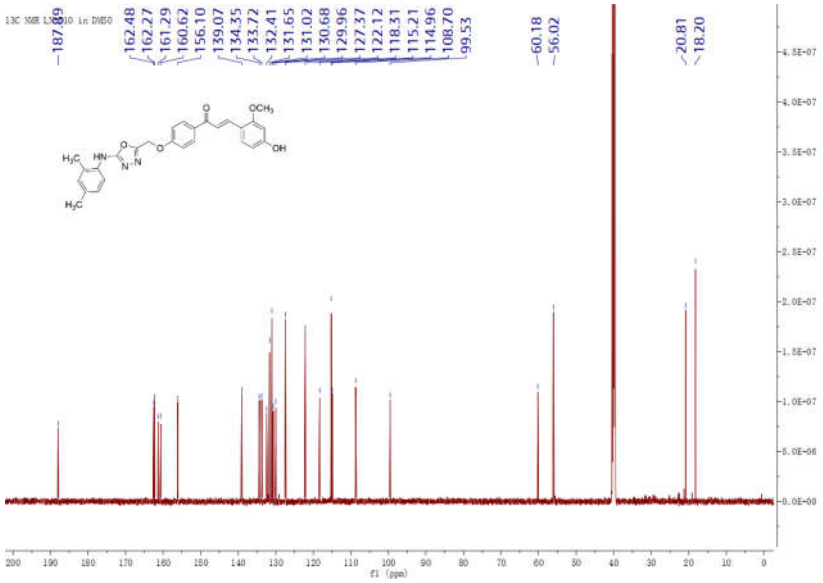

Figure S46. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T15

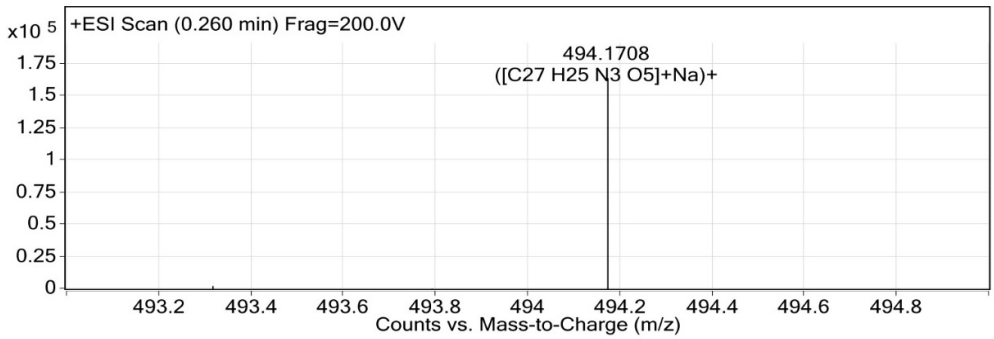

Figure S47. Mass spectrum of compound T15

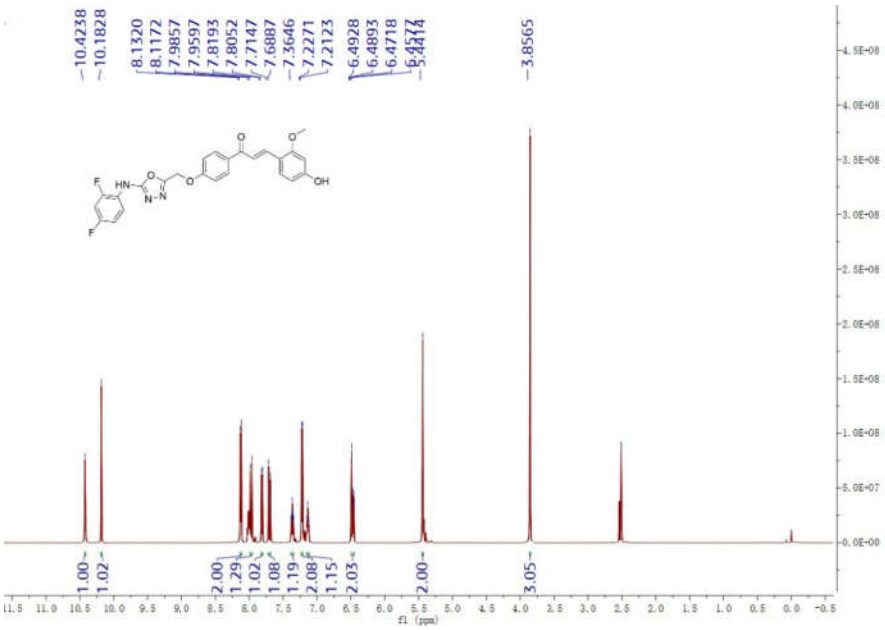

Figure S48. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T16

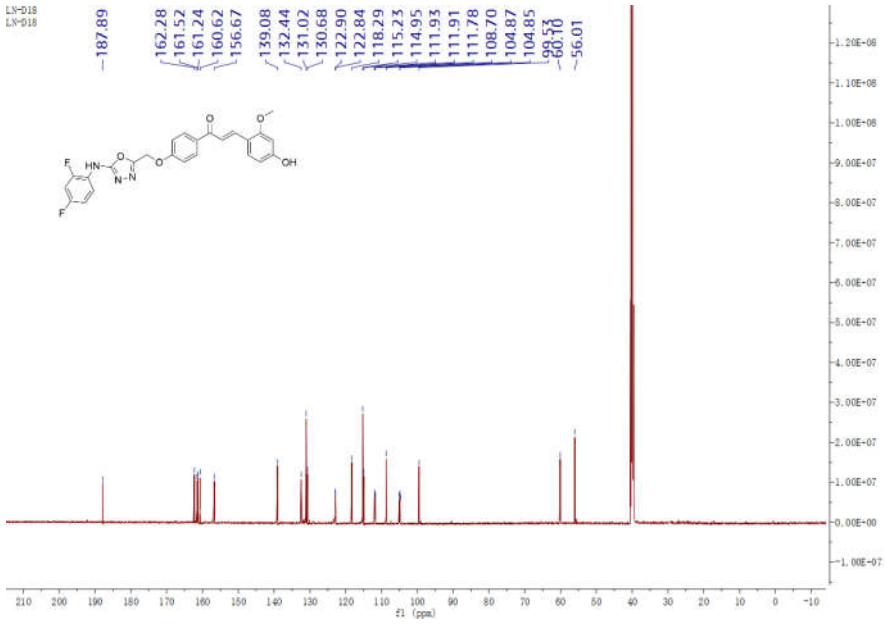

Figure S49. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T16

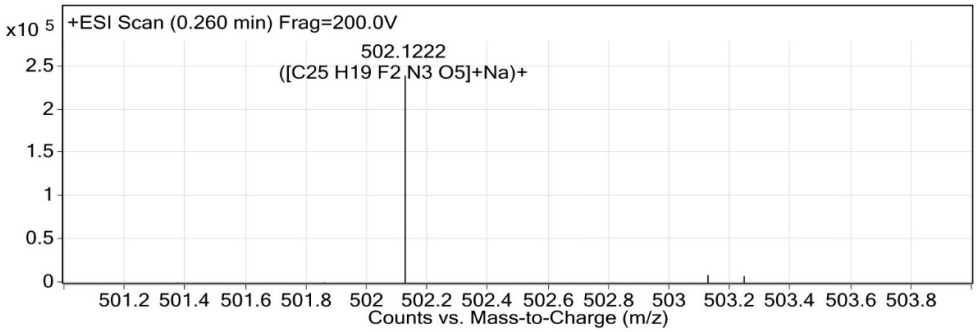

Figure S50. Mass spectrum of compound T16

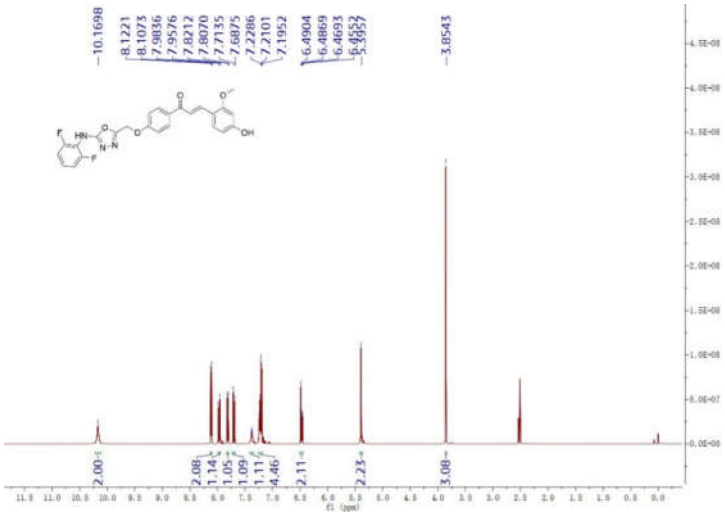

Figure S51. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T17

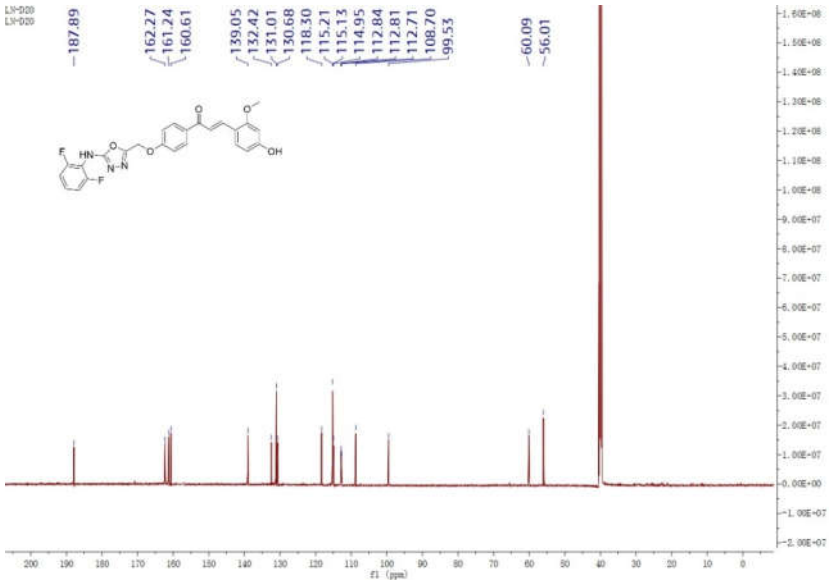

Figure S52. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound T17

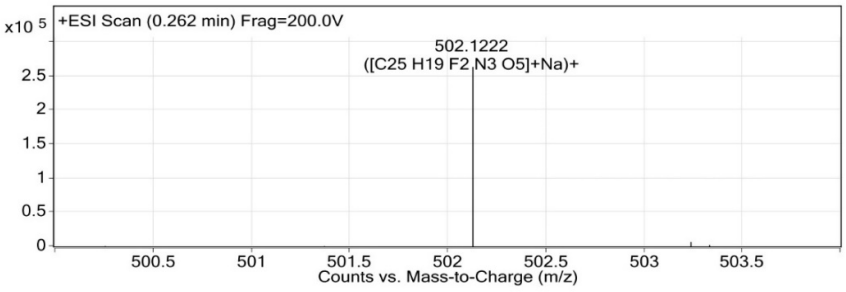

Figure S53. Mass spectrum of compound T17

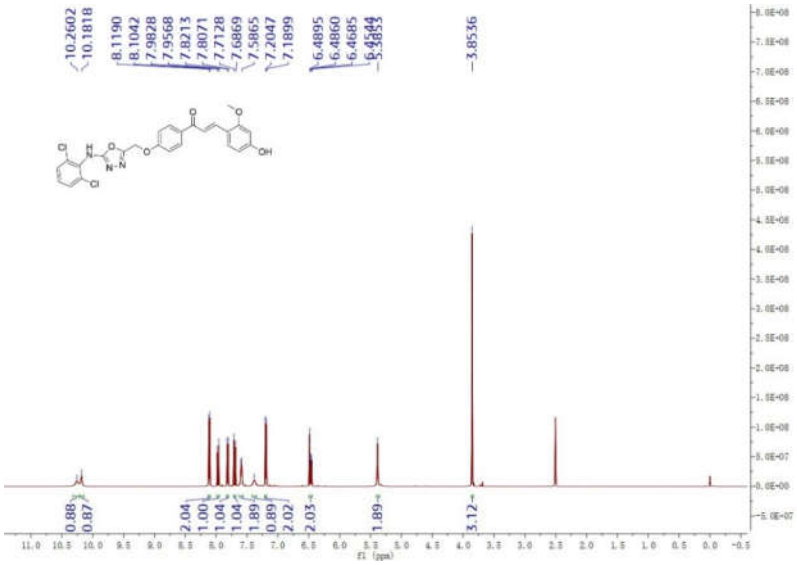

Figure S54. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of compound T18

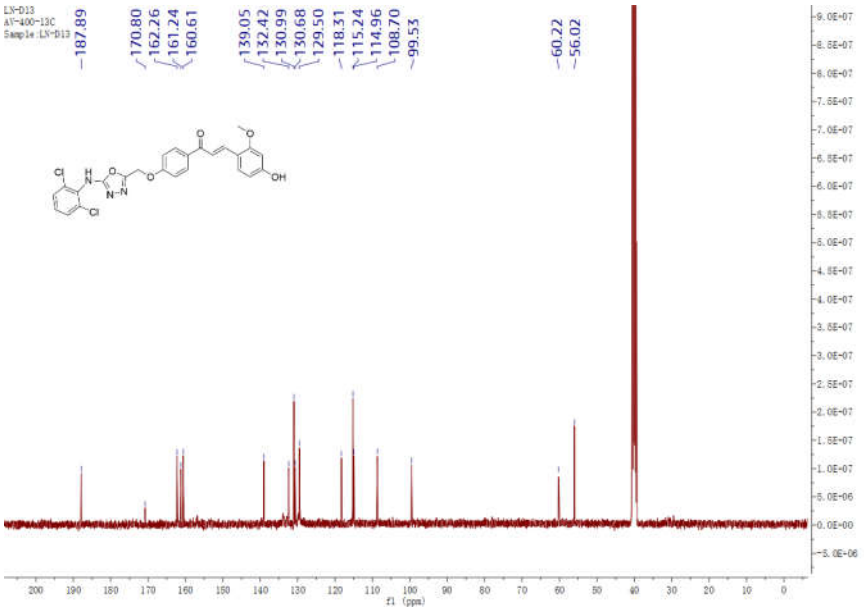

Figure S55. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of compound 18

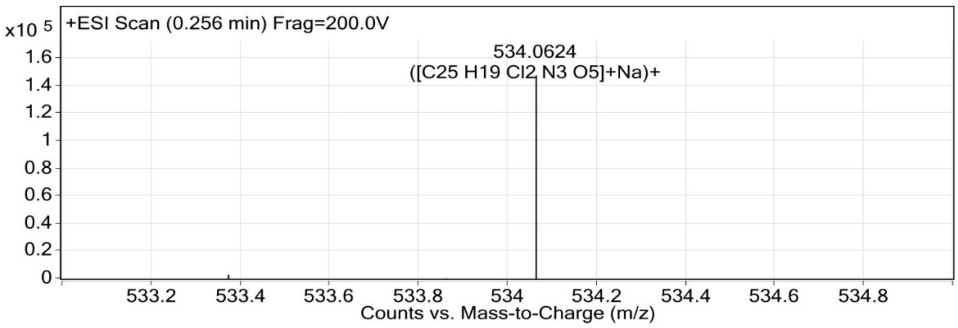

Figure S56. Mass spectrum of compound T18